AIRS/OMI Tropospheric ozone assimilation and chemical reanalysis during the NASA KORUS-AQ aircraft campaign

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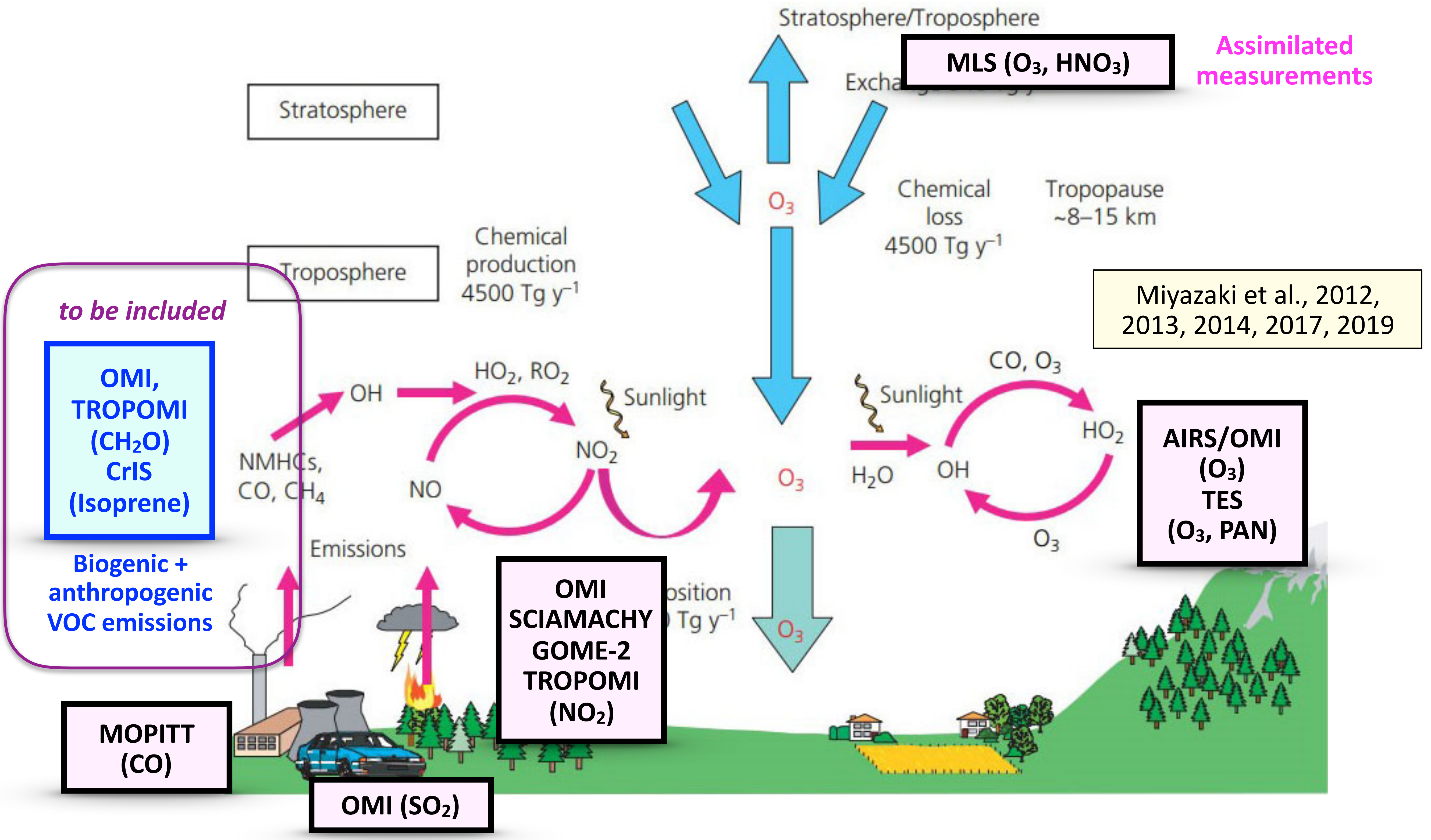
B. Gaubert, J. Barre, L. Emmons (NCAR), and KORUS-AQ team

- Fu et al., Retrievals of tropospheric ozone profiles from the synergism of AIRS and OMI: methodology and validation, Atmos. Meas. Tech., 11, 5587-5605, 2018.
- Miyazaki et al., Balance of emission and dynamical controls on ozone during the Korea-United States Air Quality campaign from multiconstituent satellite data assimilation. J. Geophys. Res., 124, 387–413, 2019

Multi-constituent satellite data assimilation using EnKF



Human activity - Air quality - Human health - Ecosystem

Simultaneously optimise chemical concentrations and emissions (NOx, CO, SO2) of various species.
Improves the representation of the entire chemistry system incl. OH, which benefits the emission estimates

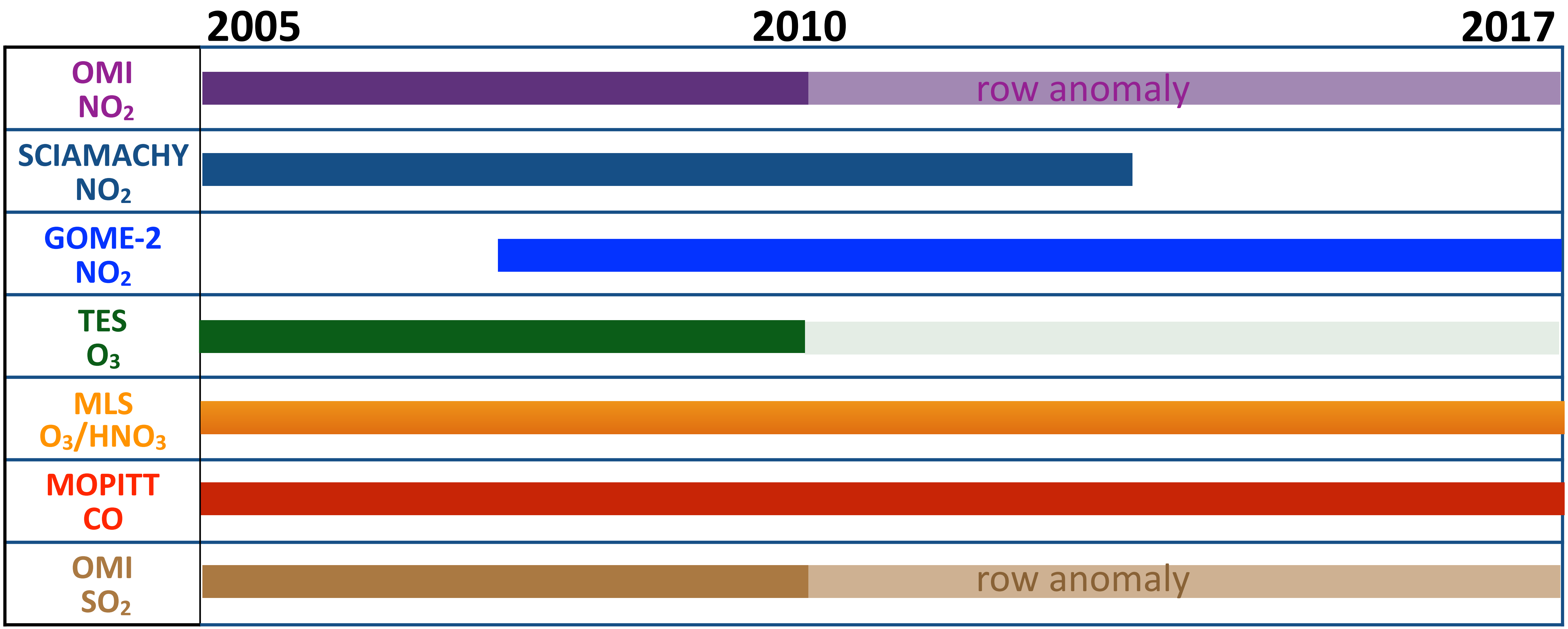
Assimilation of multiple satellite data

DA scheme	**EnKF**, 48 members
Forecast model	CHASER (MIROC-ESM) 92 species & 262 reactions for Troposphere/Stratosphere
State vector	NOx, CO, SO_2 emissions, lightning NOx, 35 chemical species
Assimilated data	OMI, SCIAMACHY, GOME-2 NO_2 (QA4ECV), OMI SO_2 (NASA PCA), TES O3 (v6), MOPITT CO (v7J), MLS O3, HNO3 (v4.2)
A priori emissions	EDGAR v4.2 (or HTAP v2), GFED v3.1, GEIA
Resolution	(horizontal) 1.1x1.1 deg (vertical) 32 layers from the surface to 4 hPa

AIRS Atmospheric Infrared Sounder OMI GOME-2 Global Ozone Monitoring Experiment SCIAMACHY MOPITT EOS MLS

Tropospheric chemistry reanalysis (TCR)

long-term global fields that are physically and chemically consistent and in agreement with individual observations



The consistent concentration and emission reanalysis data can be used to

(1) improve the understanding of the processes controlling the atmospheric environment

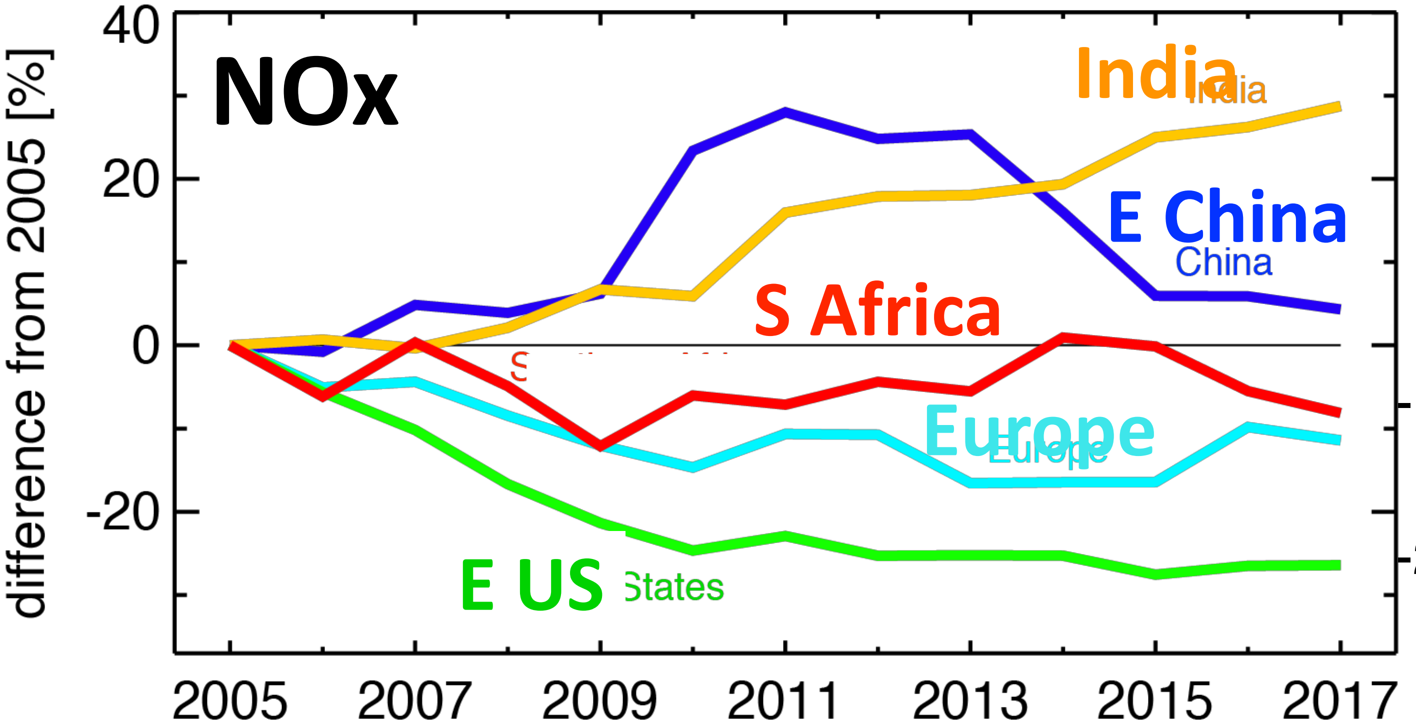
(2) provide initial and boundary conditions for climate and chemical simulations

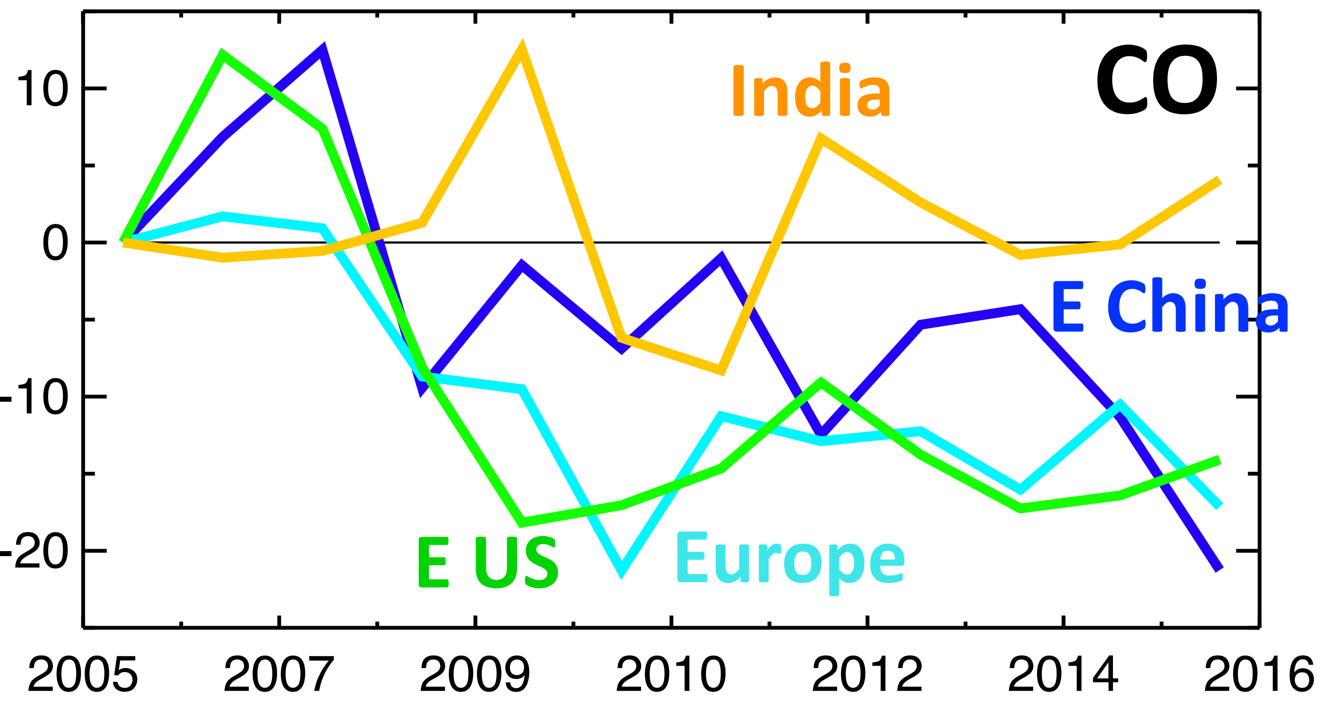
(3) evaluate models/bottom-up emission inventories

(4) suggest developments of models and observations

Global NOx and CO trends from TCR

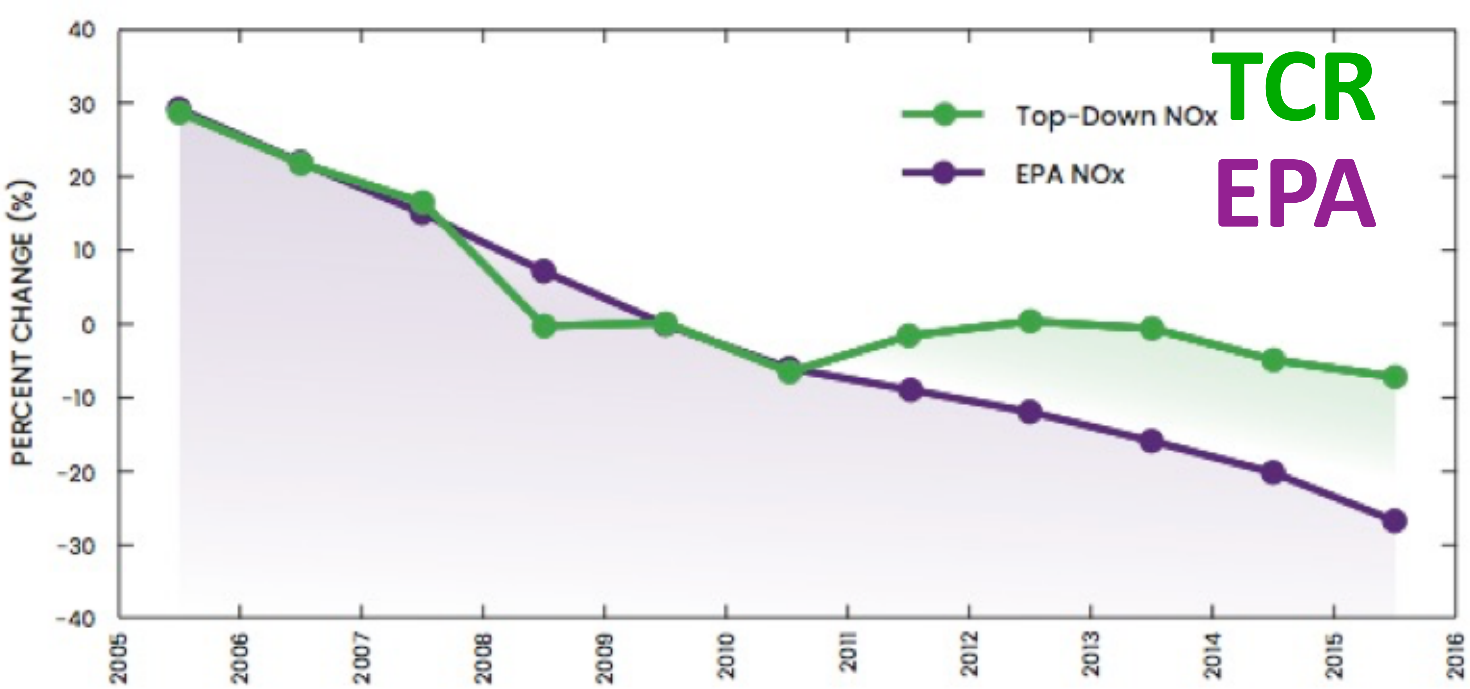
Miyazaki et al., ACP, 2017 (updated)

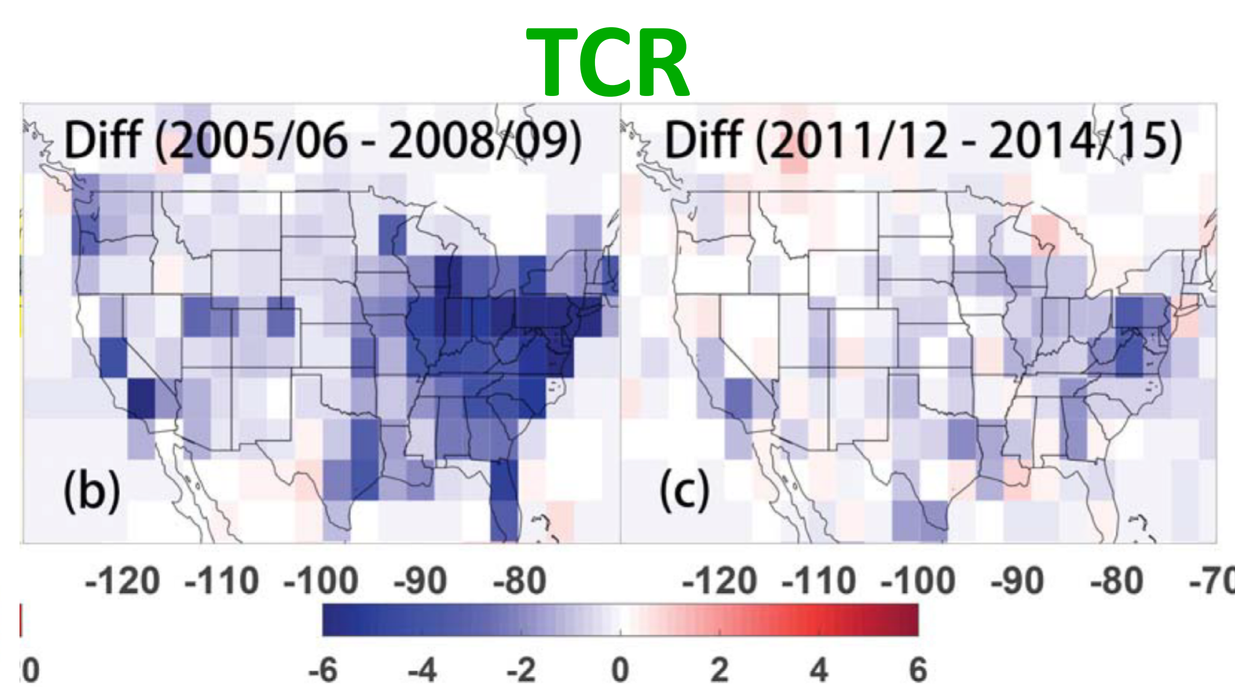




Unexpected slowdown of US pollutant emission reduction

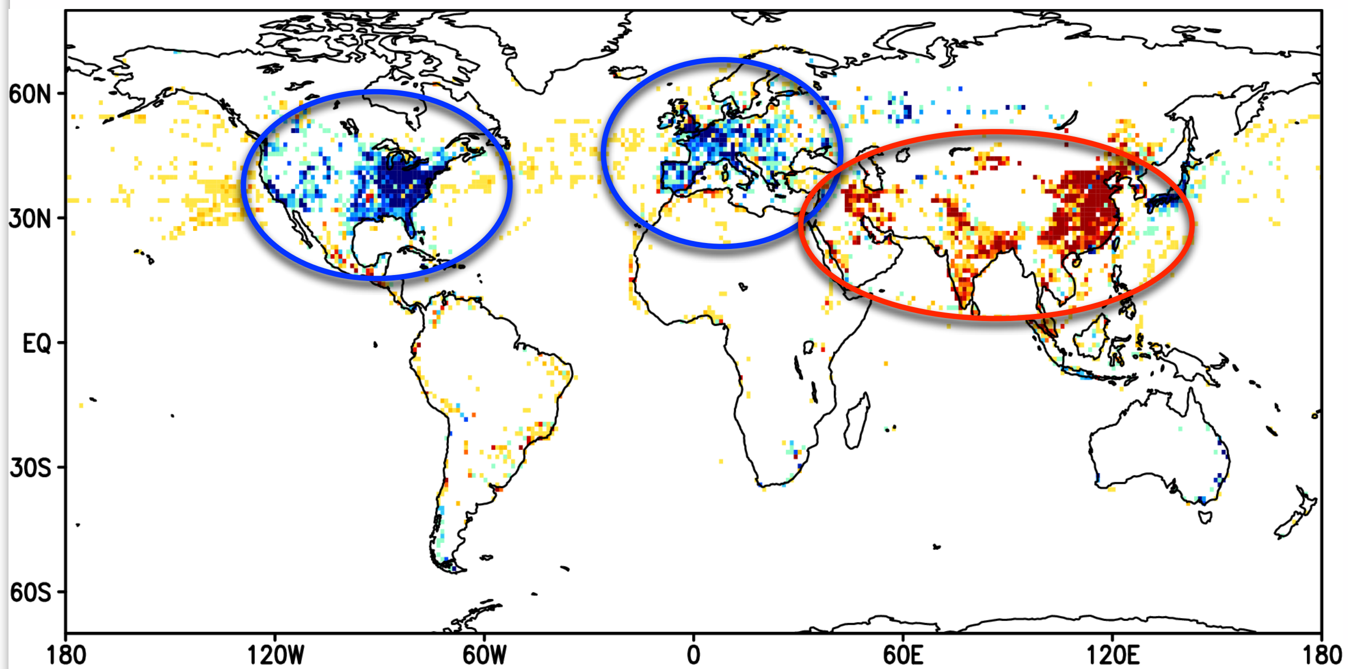
Jiang et al., PNAS, 2018



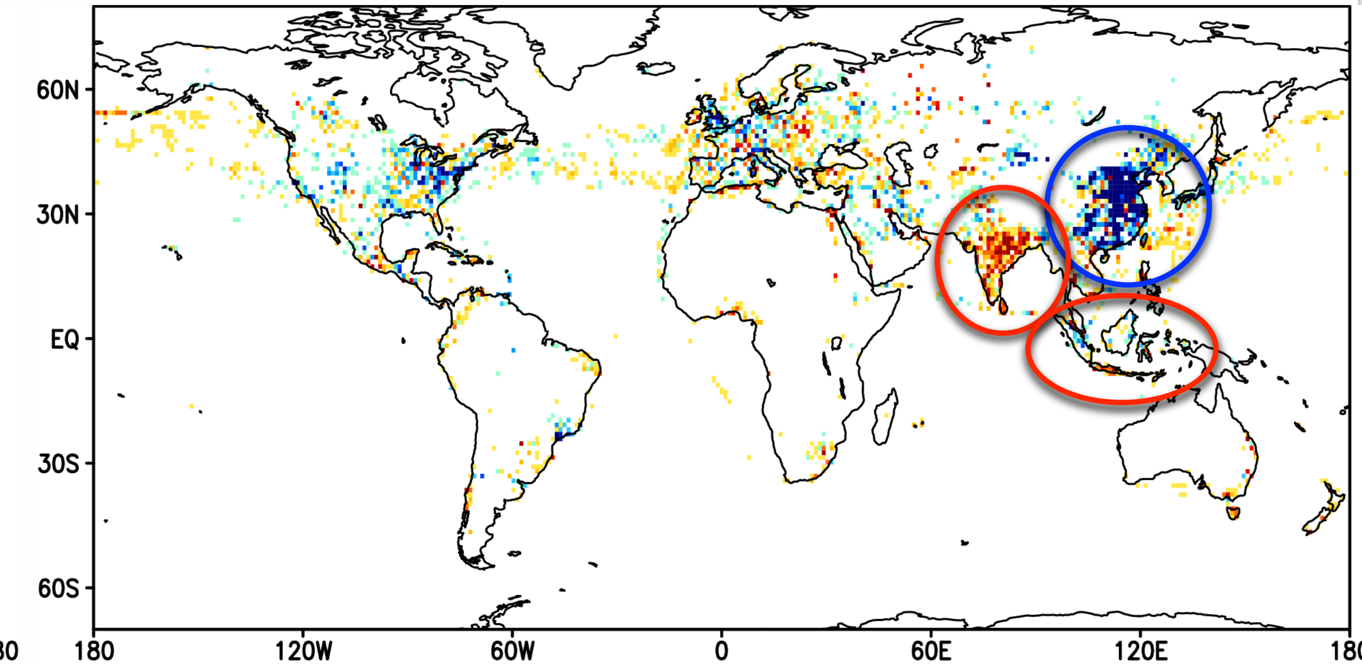


Attribution of changes in air quality

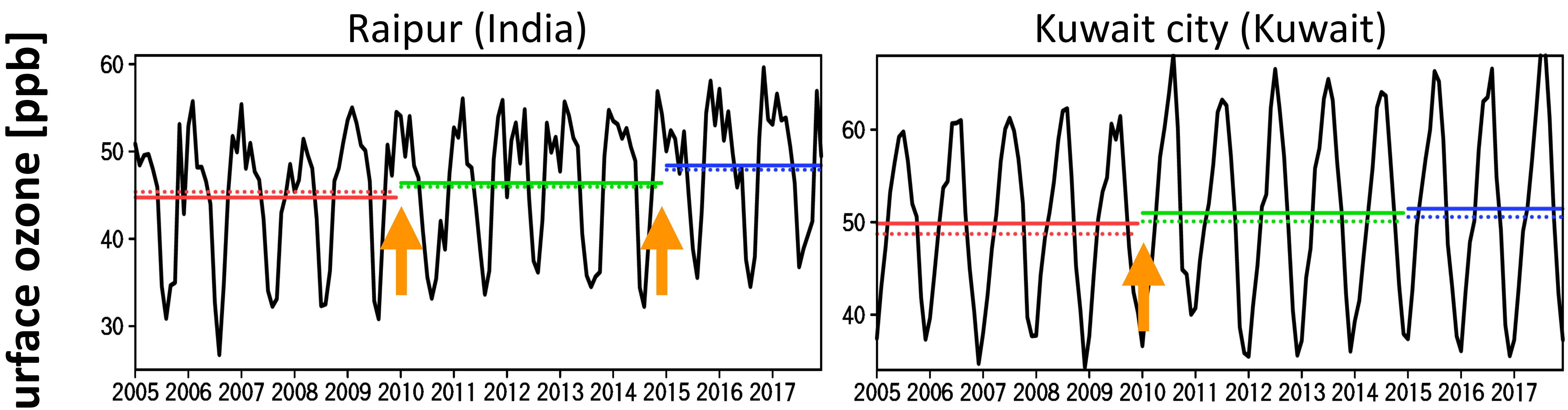
Redistribution of anthropogenic NOx emissions (economy, trade etc…)



from 2005-2009 to 2010-2014



from 2010-2014 to 2015-2017



Average 2005-2009 2010-2014 2015-2017

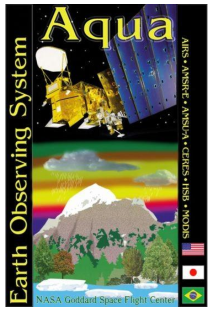
- Provides implications for air quality, human health, and ecosystem
- Would require long-term tropospheric ozone data for further improvements

Tropospheric Ozone Profile Maps from the Synergic Observation of AIRS and OMI:

Updates on Validation and Science Application for KORUS-AQ

Dejian Fu[1], Kevin W. Bowman[1], Kazuyuki Miyazaki[2], Susan S. Kulawik[1,3], John R. Worden[1], Bradley R. Pierce[4], Robert L. Herman[1], Gregory B. Osterman[1], Fredrick W. Irion[1], with thanks to KORUS-AQ, TES, AIRS, OMI, and CrIS teams

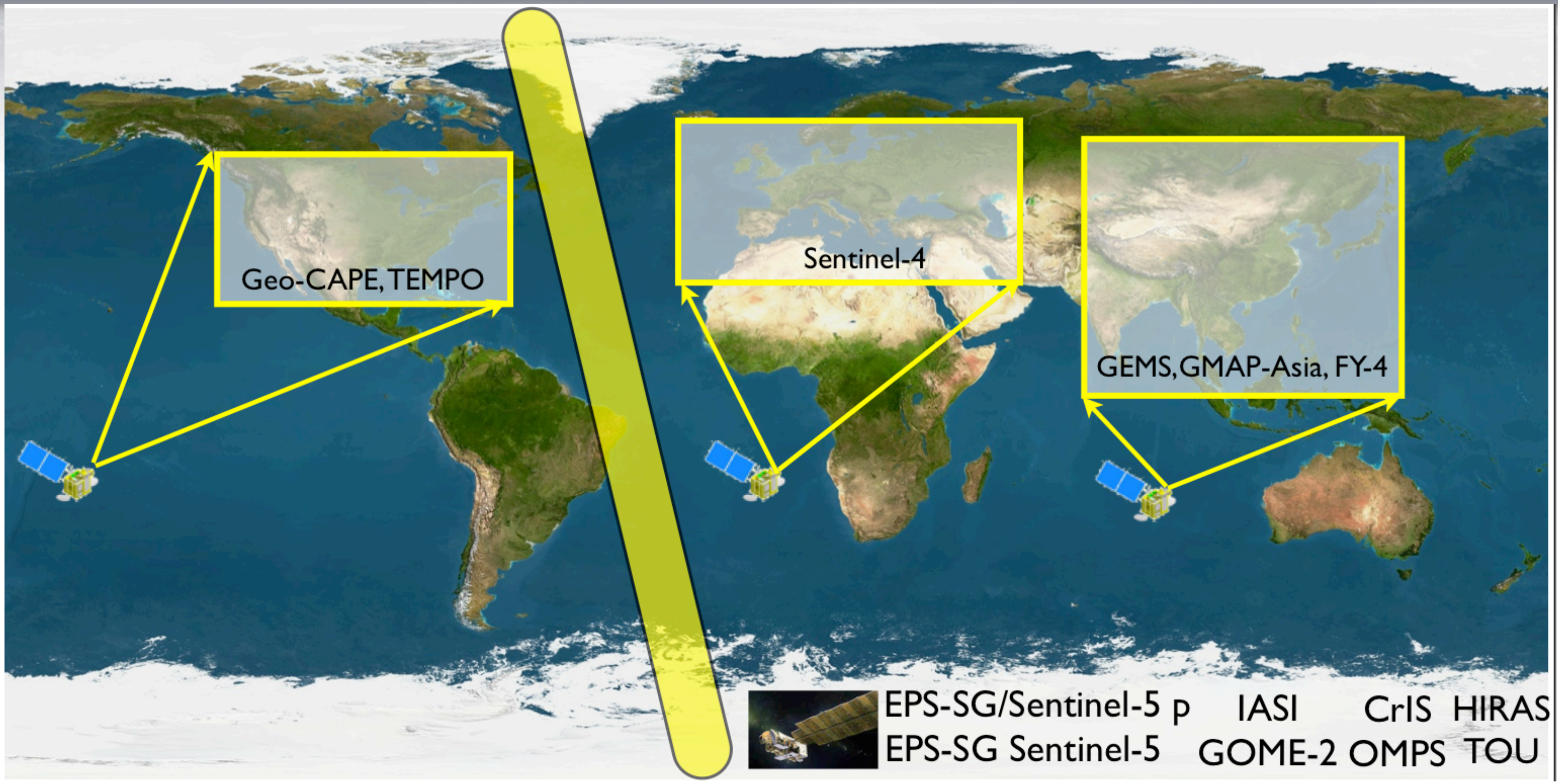
01 NASA Jet Propulsion Laboratory, California Institute of Technology, USA
02 Japan Agency for Marine-Earth Science and Technology, Japan
03 NASA Ames Research Center, USA
04 NOAA/NESDIS Center for Saellite Applications and Research, USA



Joint LW/SW or ultra-high spectral resolution measurements distinguish upper/lower troposphere

- TIR observations are sensitive to the free-tropospheric trace gases.
- UV-Vis-NIR observations are sensitive to the column abundances of trace gases.

Towards an Air Quality Constellation



Bowman, *Atm. Env.* 2013

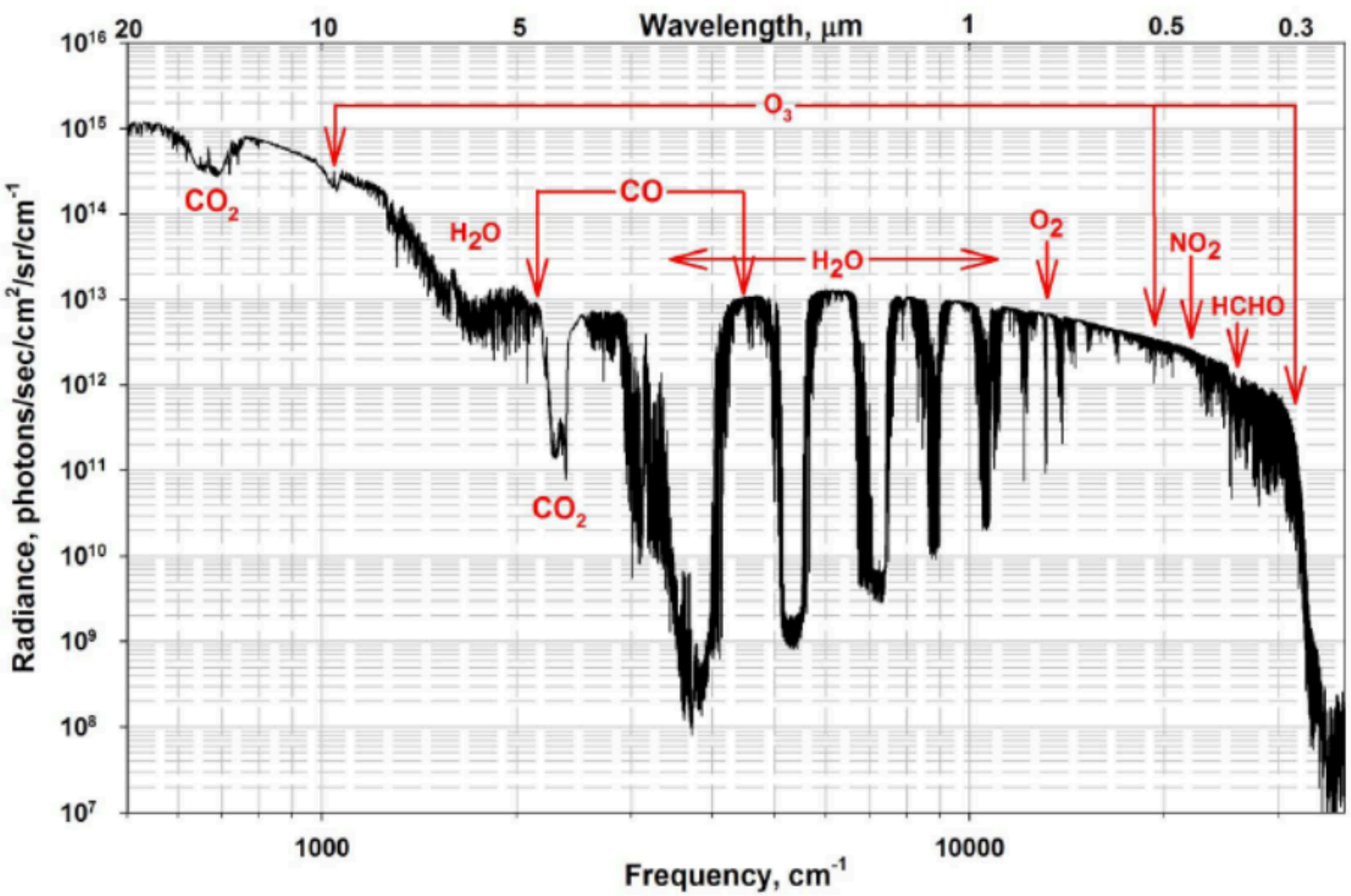
How does the constellation improve knowledge of global air quality?

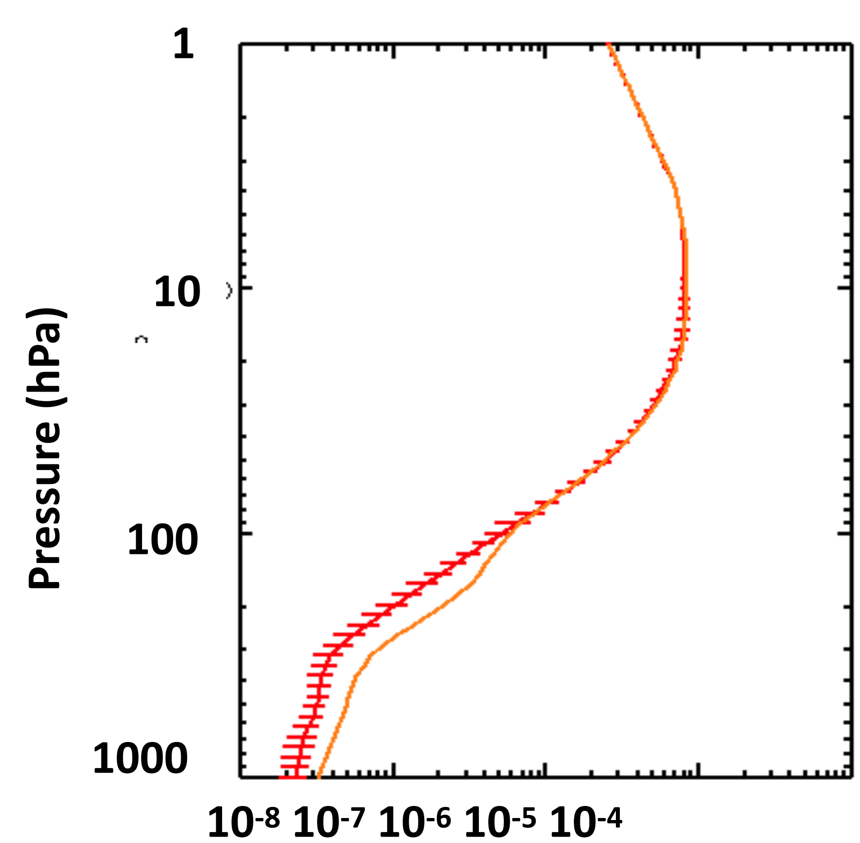
- GEO sounders (GEO-CAPE, TEMPO, Sentinel-4, GEMS) will provide an unprecedented number of composition observations at high spatial resolution.
- LEO sounders (IASI, CrIS, S5p) provide the global picture and thread the GEO observations together.

The Synergic Observations

Joint LW/SW or ultra-high spectral resolution measurements distinguish upper/lower troposphere.

- TIR observations are sensitive to the free-tropospheric trace gases.
- UV-Vis-NIR observations are sensitive to the column abundances of trace gases.

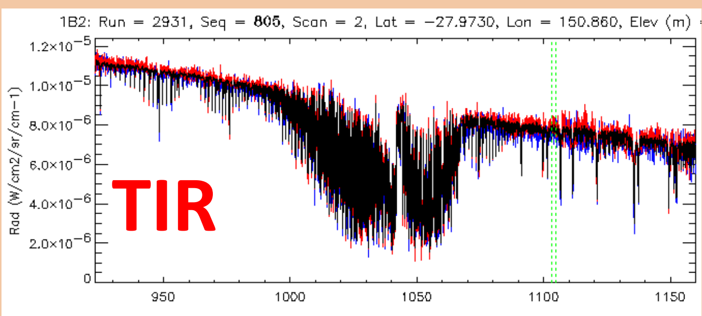


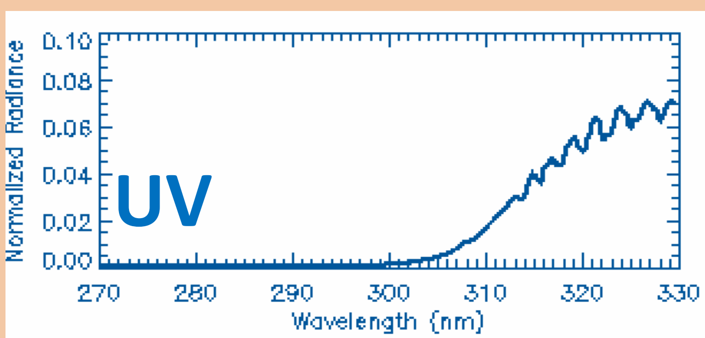


MUlti-SpEctra, MUlti-SpEcies, MUlti-SEnsors (MUSES) Retrieval Algorithm

Connecting Remote Sensing to Assimilation

JPL MUSES algorithm delivers both retrieved trace gas concentration profiles and observation operators needed for trend analysis, climate model evaluation, and data assimilation.

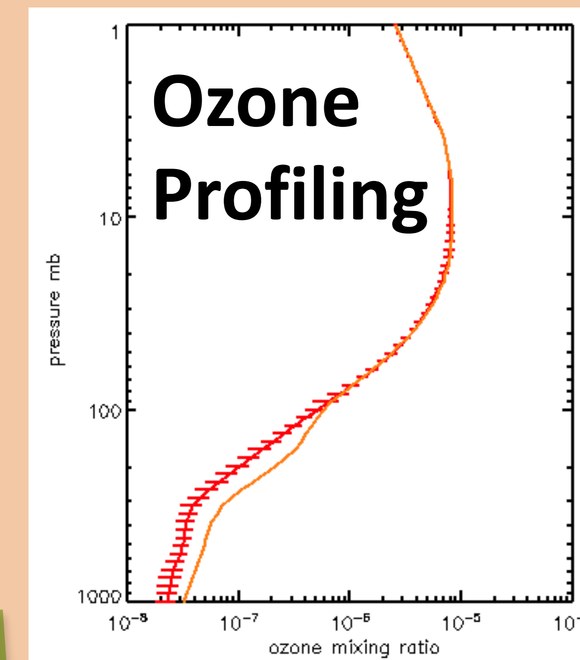




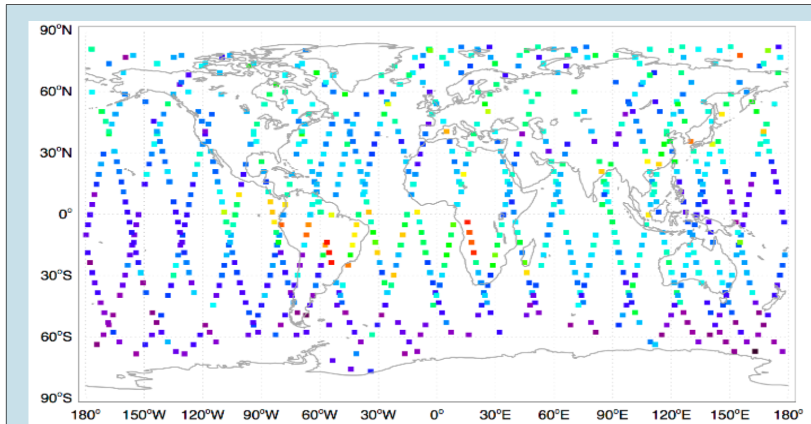
$$\|\mathbf{y}-\mathbf{F}(\mathbf{x}_a)\|^2_{\mathbf{S}_n^{-1}} + \|\mathbf{x}-\mathbf{x}_a\|^2_{\mathbf{S}_a^{-1}}$$

NASA Retrieval Algorithm

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}(\mathbf{x}-\mathbf{x}_a) + \mathbf{G}\mathbf{n}$$

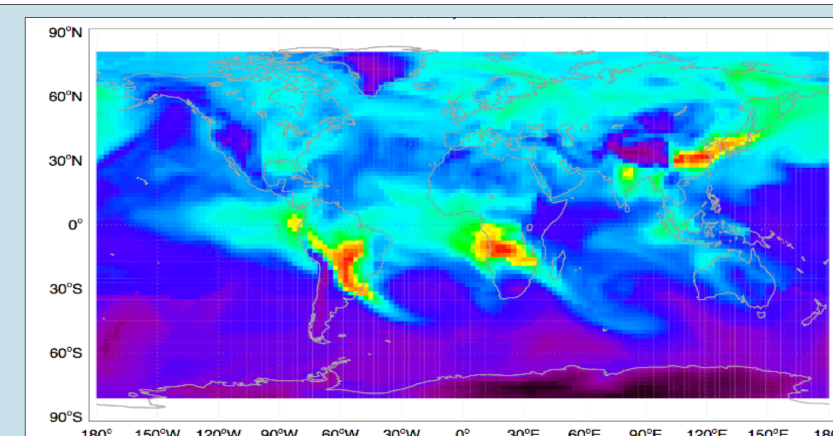


Operational Data Processing



JAMSTEC
Data Assimilation

$$\mathbf{H}_i(\bullet) = \mathbf{x}_a + \mathbf{A}_i(\bullet - \mathbf{x}_a)$$



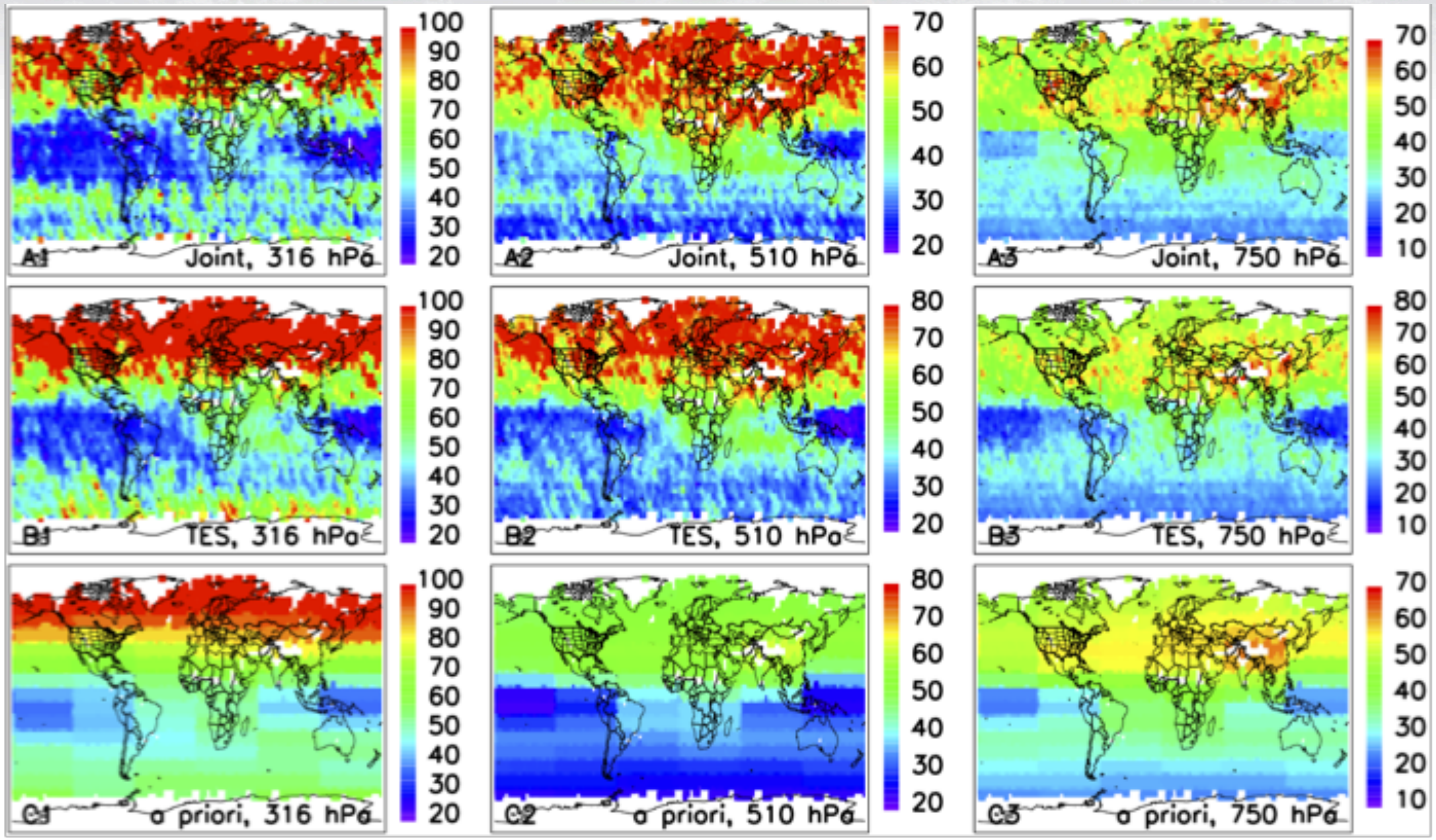
$$\sum_i \|\hat{\mathbf{x}}_i - \mathbf{H}_i(\mathbf{x})\|^2_{(\mathbf{G}_i\mathbf{S}_n^i\mathbf{G}_i^T)^{-1}} + \|\mathbf{x}_0 - \mathbf{x}_B\|^2_{\mathbf{B}^{-1}}$$

Joint AIRS+OMI O_3 vs. TES Global Survey Mode

Joint AIRS/OMI

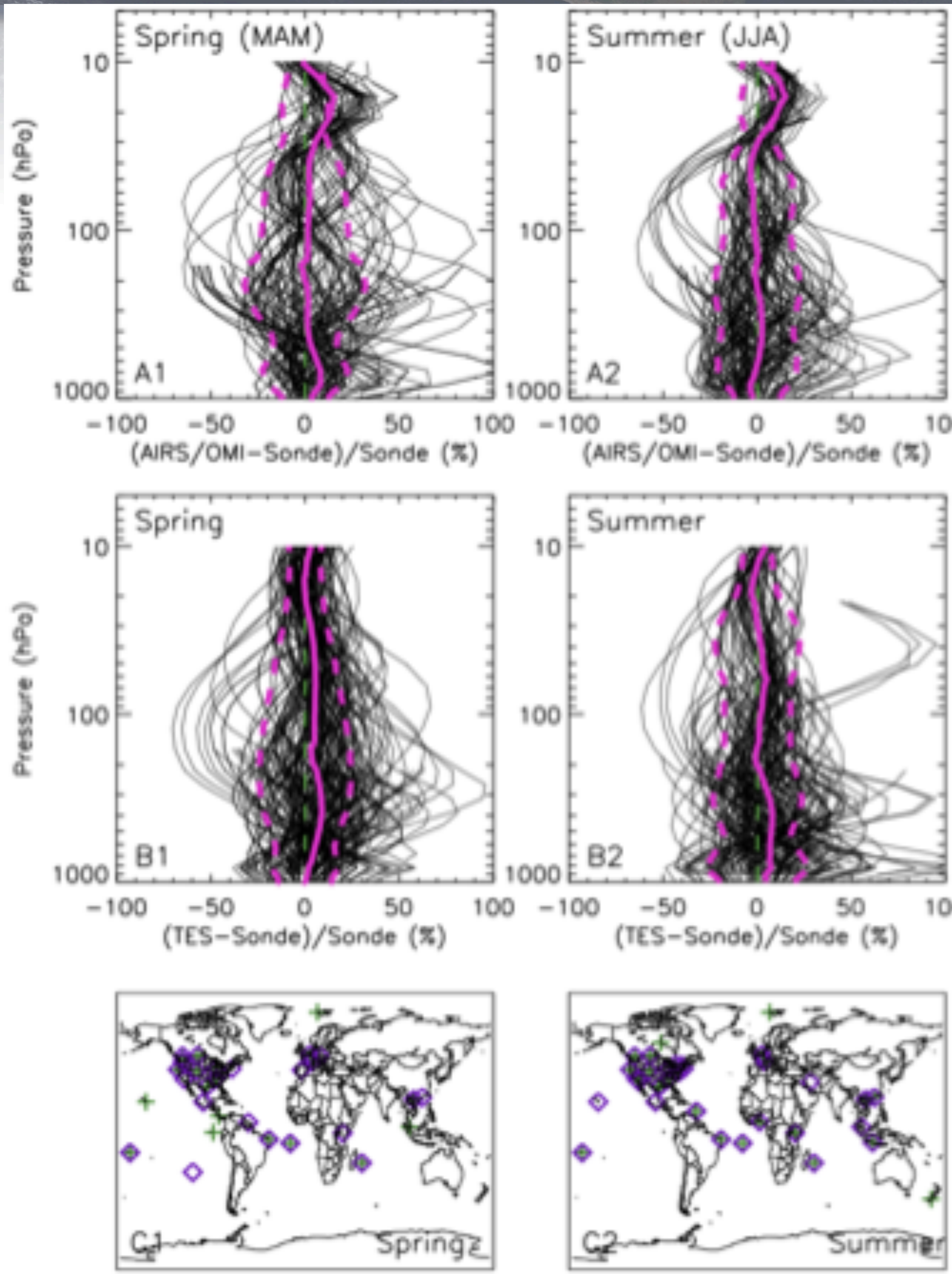
TES version 6.0

A priori



- The correlation coefficients of joint AIRS+OMI vs. TES ozone data: 0.71 - 0.92 for all months.
- The characteristics of the joint AIRS+OMI retrievals, in terms of vertical sensitivity and estimated uncertainty characteristics, are equivalent to those of TES data.

Comparisons to WOUDC Ozonesondes



	316 hPa	Spring	
		AIRS+OMI	TES
	Mean (ppb)	2.8	6.1
	Mean (%)	1.3	8.6
	RMS (ppb)	17.1	19.2
	RMS (%)	25.6	23.7
Differences (Satellite – WOUC Sonde with Satellite Observation Operator Applied)	510 hPa	Spring	
		AIRS+OMI	TES
	Mean (ppb)	1.3	3.6
	Mean (%)	3.8	7.0
	RMS (ppb)	7.6	9.2
	RMS (%)	17.2	17.4
	750 hPa	Spring	
		AIRS+OMI	TES
	Mean (ppb)	2.4	1.7
	Mean (%)	8.0	3.4
	RMS (ppb)	7.6	6.9
	RMS (%)	21.1	16.2
Number of WOUDC Sonde Sites		20	25
Number of Satellite/Sonde Coincidences		131	197

Coincident criteria

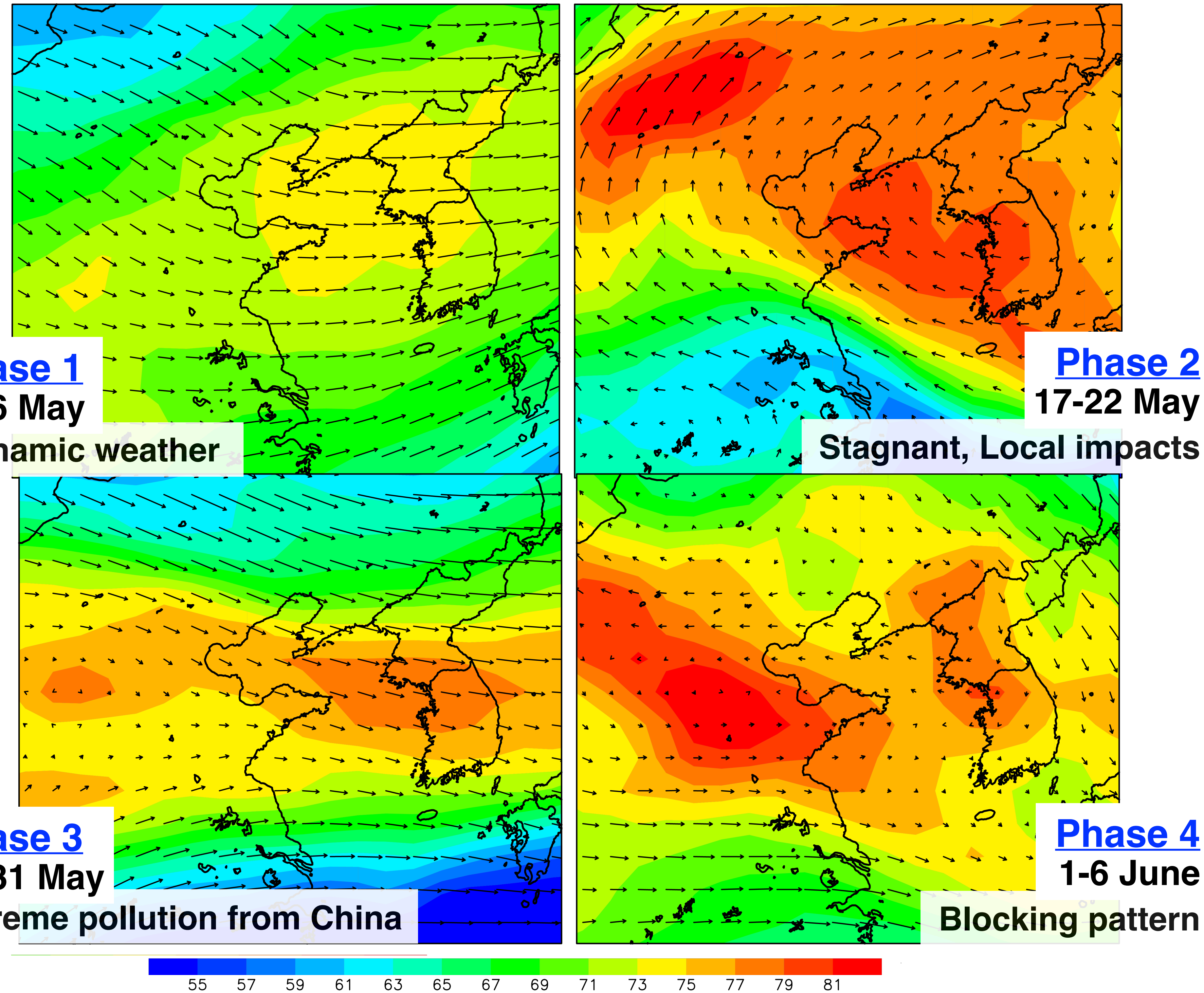
- Passed retrieval quality check
- Distance < 300 km; Time diff. < 4 hours
- Day Time
- Cloud optical depth < 2.0

Chemical reanalysis and AIRS/OMI ozone applications for the NASA KORUS-AQ aircraft campaigns

Reanalysis ozone at 700 hPa

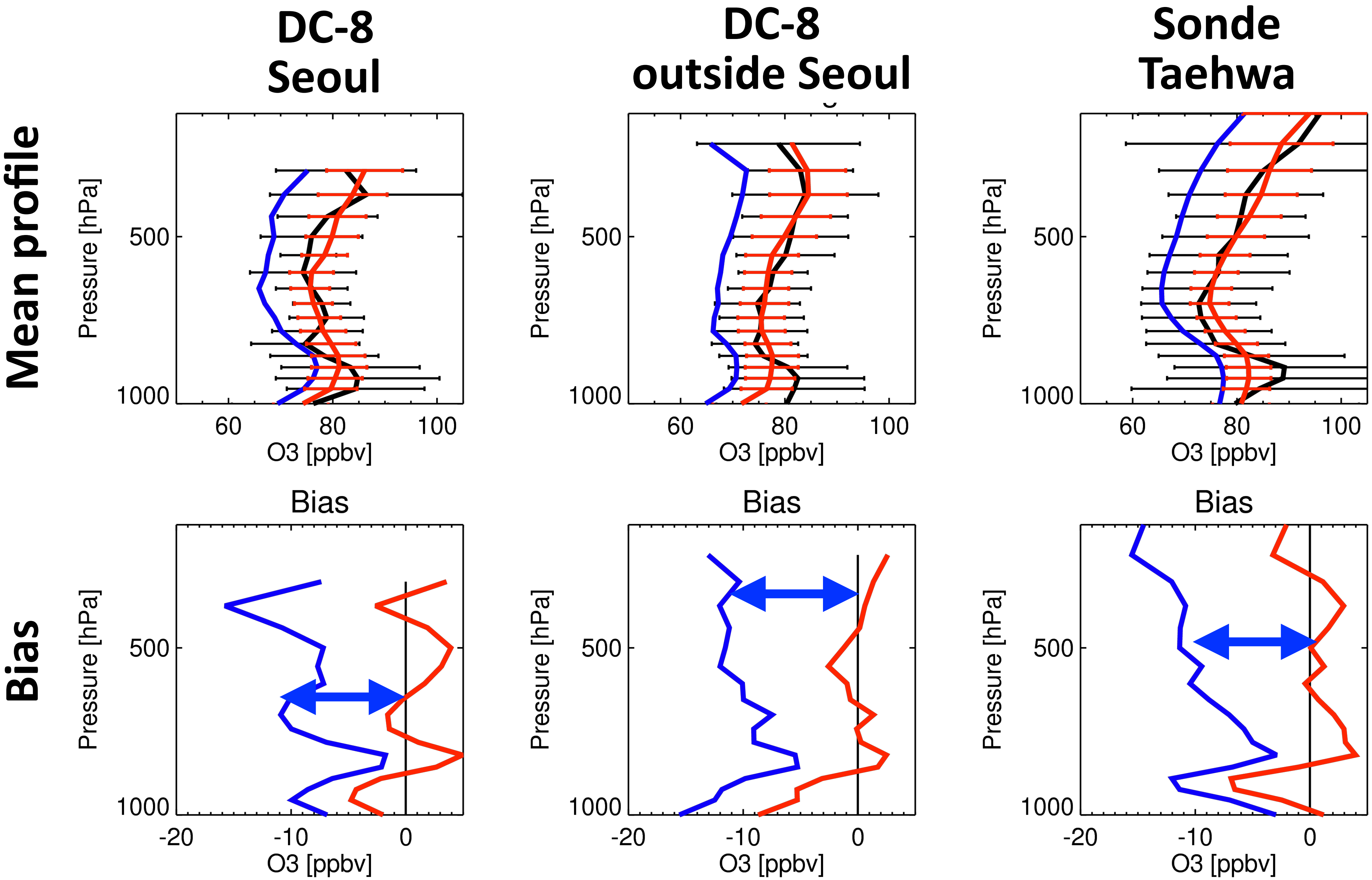
May-Jun 2016
South Korea

Ministry of Environment
National Institute of Environmental Research



persistently higher over Seoul (76.0±7.9ppbv) than over the broader domain (70.9±9.4ppbv)

Chemical reanalysis and AIRS/OMI ozone applications for the NASA KORUS-AQ aircraft campaigns



O_3 profiles

Observation
Model
Reanalysis

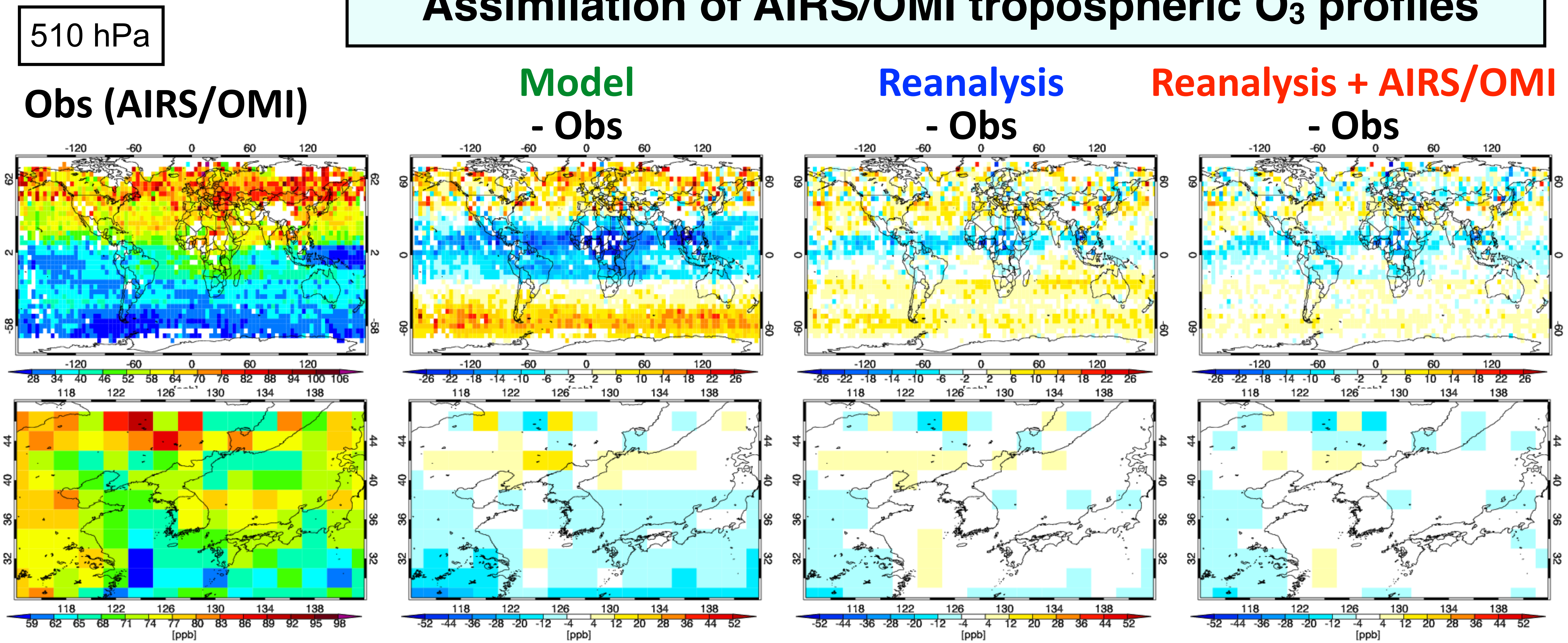
Model bias: 10-20 ppb

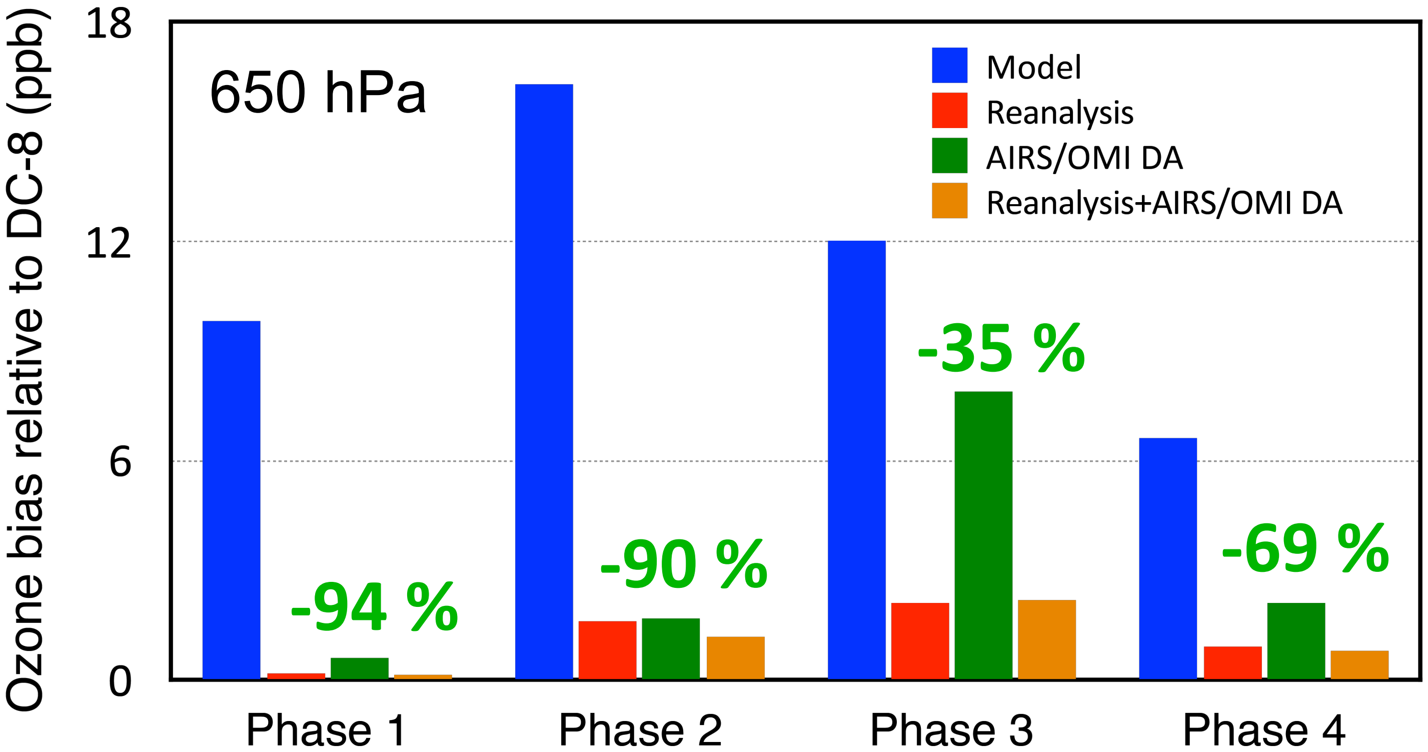
<u>Analysis bias < 5 ppb</u>
none of tropospheric O_3 obs was assimilated!

+ new AIRS/OMI products from the NASA JPL MUSES algorithm

could help further improve the ozone analysis and in the quantitative attribution of anthropogenic emissions and natural influences of pollutants.

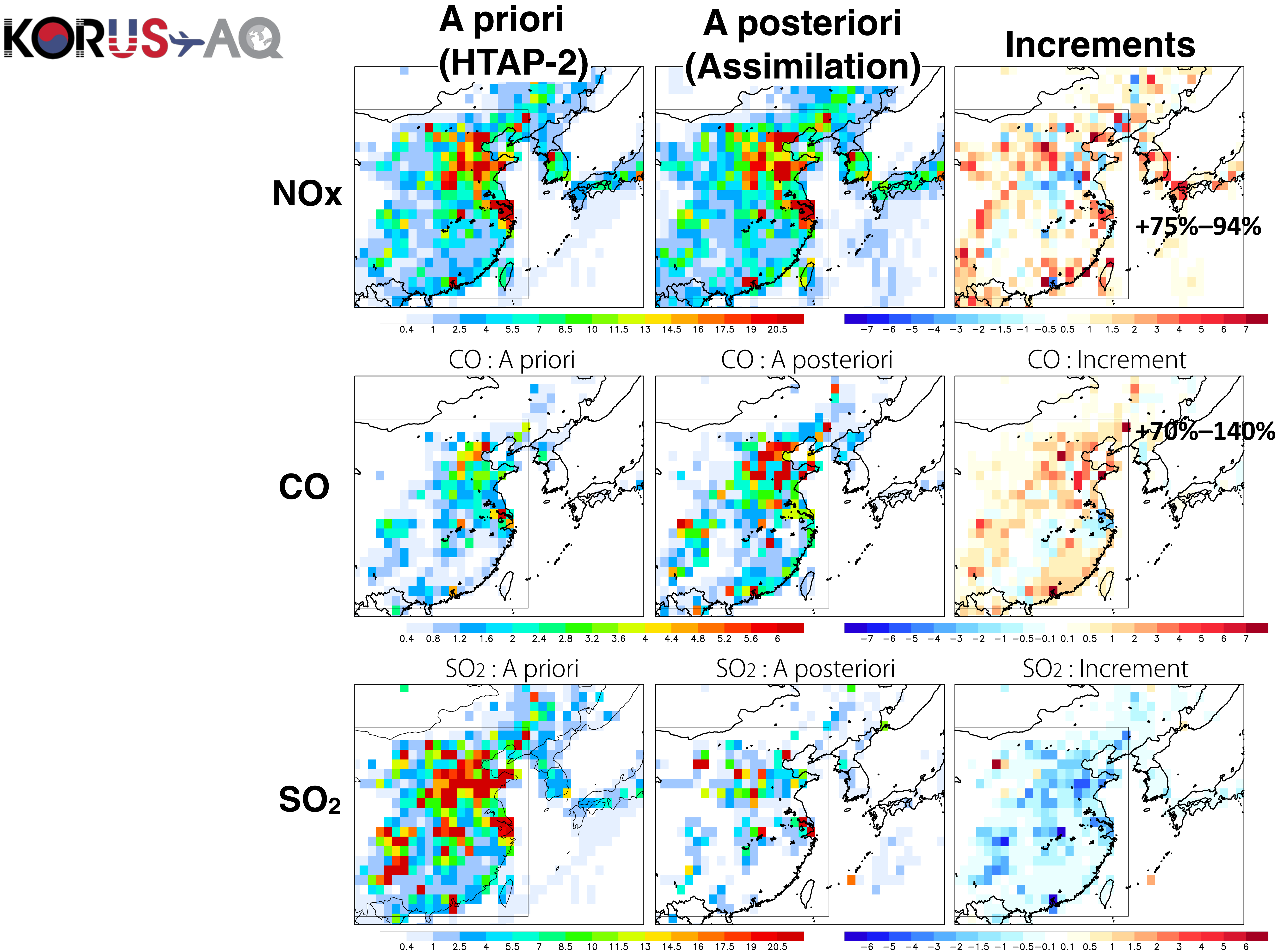
Assimilation of AIRS/OMI tropospheric O_3 profiles



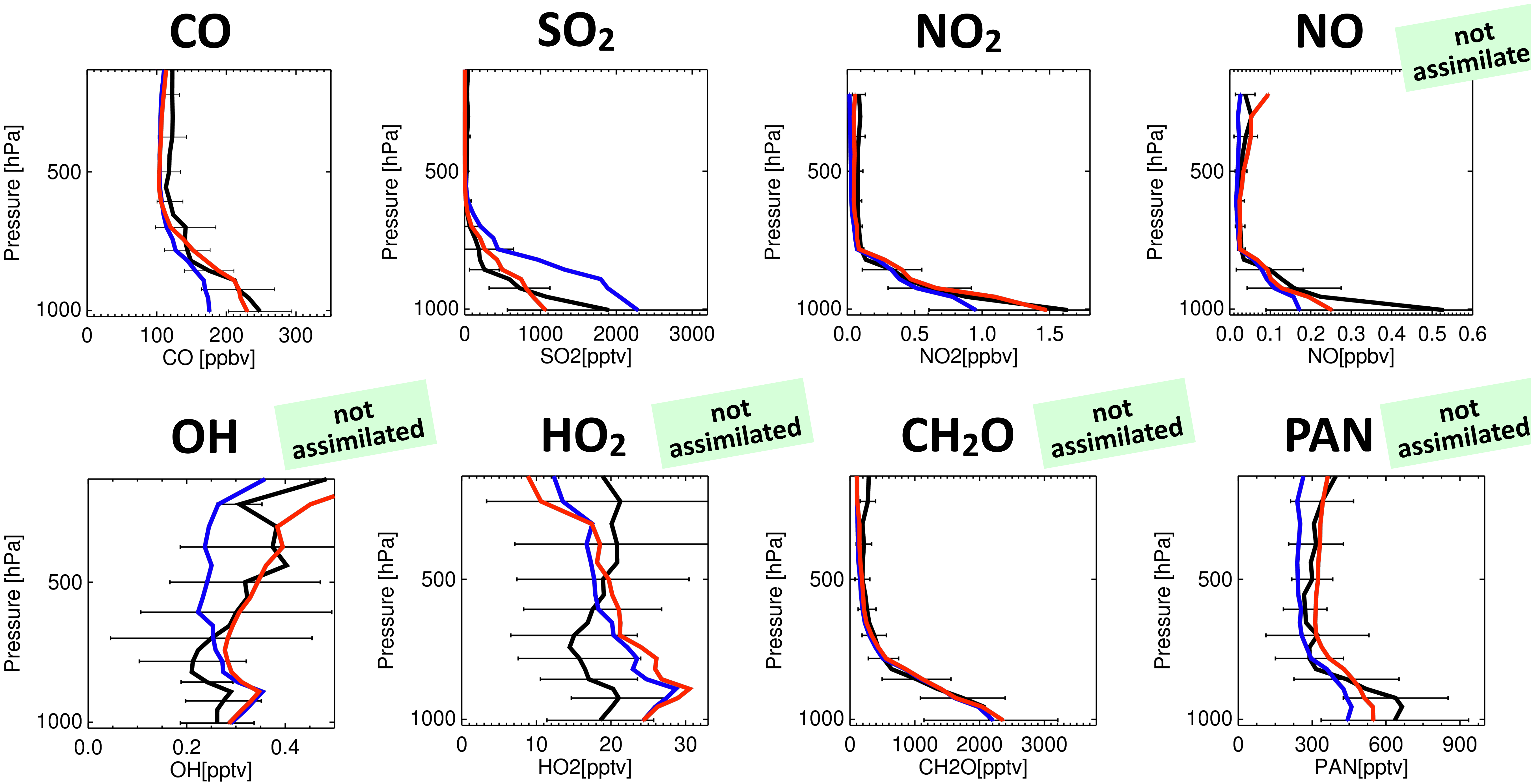


Comparisons against KORUS-AQ DC8 ozone

- Assimilation of AIRS/OMI retrievals provided the largest corrections for dynamic weather conditions (P1), whereas the improvement was limited just after stagnant conditions (P3).
- Combining precursors' emission optimization and direct ozone assimilation is an effective method to obtain sufficient corrections on ozone for any meteorological condition.


KORUS-AQ
A priori (HTAP-2)
A posteriori (Assimilation)
Increments
NOx
+75%–94%
0.4 1 2.5 4 5.5 7 8.5 10 11.5 13 14.5 16 17.5 19 20.5
−7 −6 −5 −4 −3 −2 −1.5 −1 −0.5 0.5 1 1.5 2 3 4 5 6 7
CO : A priori
CO : A posteriori
CO : Increment
CO
+70%–140%
0.4 0.8 1.2 1.6 2 2.4 2.8 3.2 3.6 4 4.4 4.8 5.2 5.6 6
−7 −6 −5 −4 −3 −2 −1 −0.5 −0.1 0.1 0.5 1 2 3 4 5 6 7
SO2 : A priori
SO2 : A posteriori
SO2 : Increment
SO2
0.4 1 2.5 4 5.5 7 8.5 10 11.5 13 14.5 16 17.5 19 20.5
−6 −5 −4 −3 −2 −1.5 −1 −0.5 −0.1 0.1 0.5 1 1.5 2 3 4 5 6

KORUS-AQ



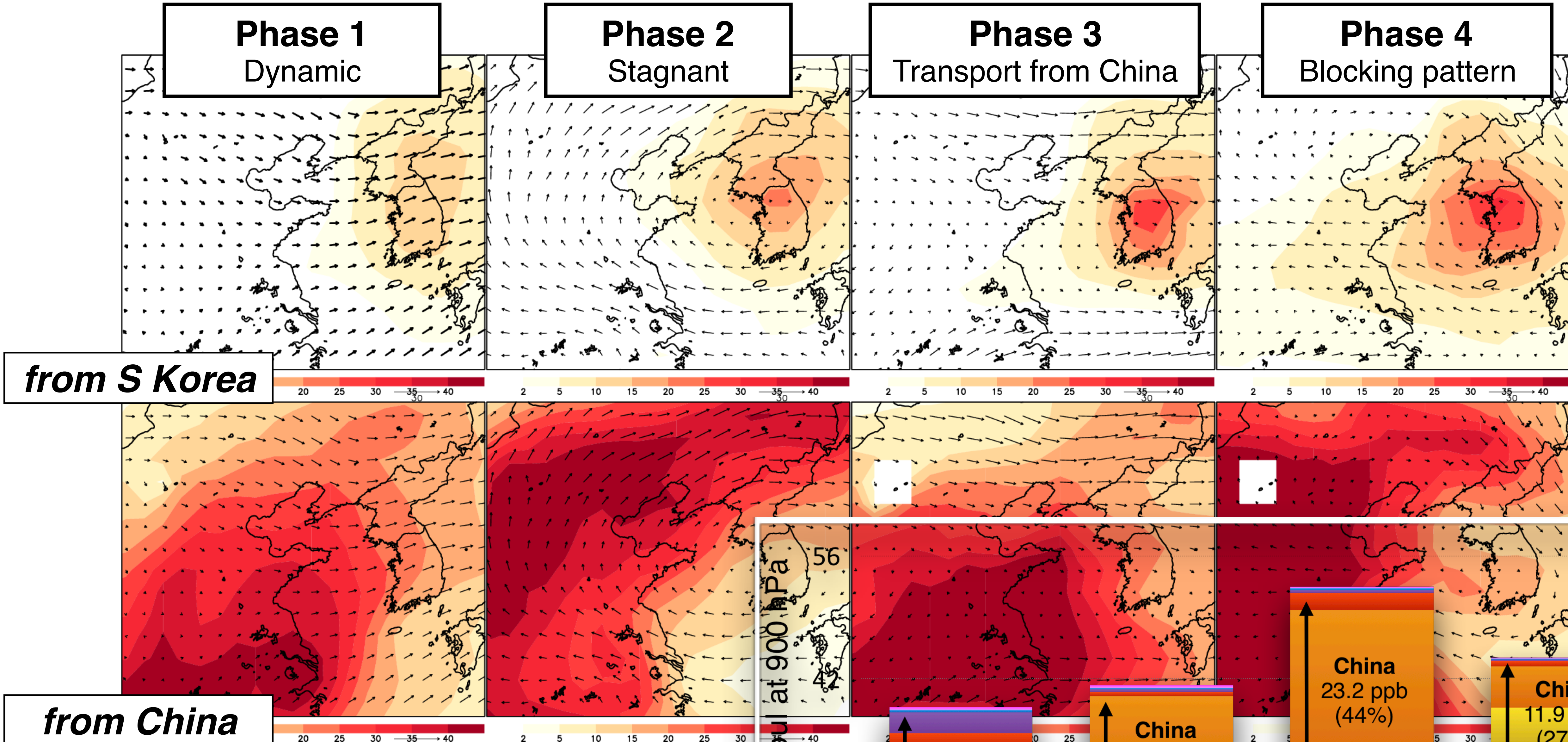
DC-8 profiles outside Seoul

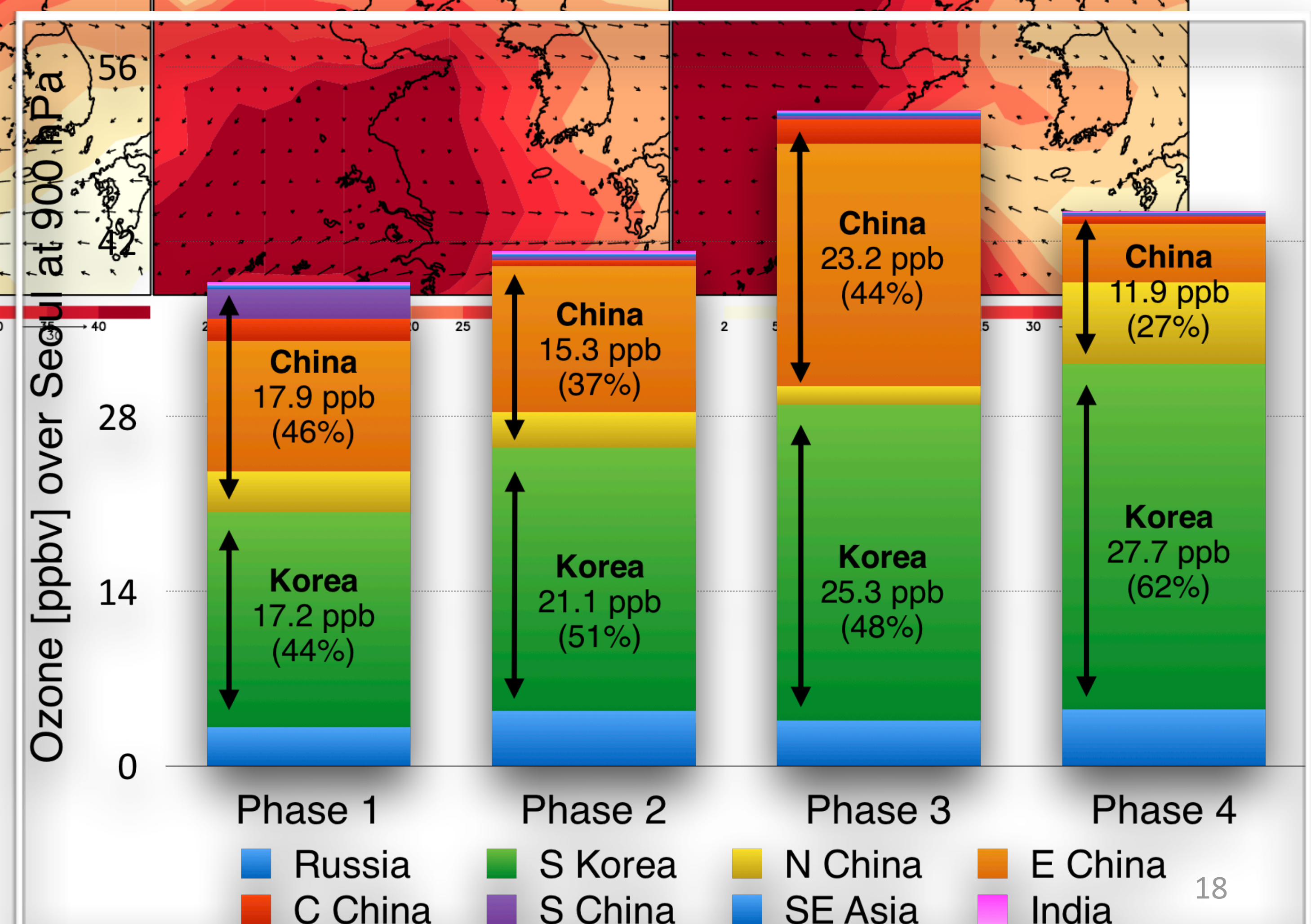
Observation
Model
Reanalysis

The multiple-species DA provides comprehensive constrains on the tropospheric chemistry system

Source-receptor analysis

900 hPa ozone





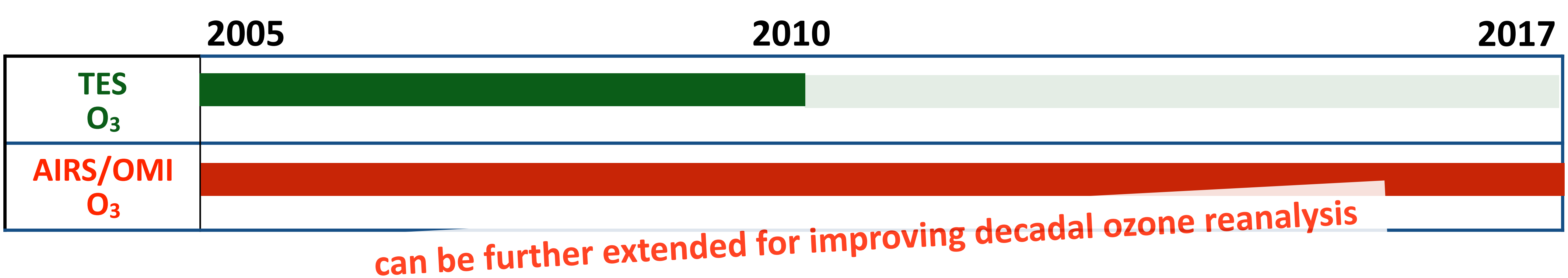
- Korean emissions: up tp 13 ppm (P2)
- Chinese emissions: up to 23 ppb (P3)

Data Processing of Joint AIRS/OMI O_3 Retrievals

The AIRS/OMI retrievals have been configured in two modes: global survey (GS) & regional mapping (RE).

- **GS mode**
  - Provides profile data with a spatial sampling similar to TES global survey
    - ✓ **Year 2006, 2007, 2008**
    - ✓ **March-June 2016**
    - ✓ **December 2017 to present**
  - GS data are available via the link (AIRS-OMI combined products) at https://tes.jpl.nasa.gov/data/
- **RE mode**
  - Processes all available measurements for flight campaigns including
    - ✓ **KORUS-AQ, Apr – Jun 2016**
    - ✓ ORACLES, Aug, Sept 2016
    - ✓ POSIDON, Sept, Oct 2016
  - **KORUS-AQ (Apr-June 2016) RE** data are available at https://tes.jpl.nasa.gov/data/

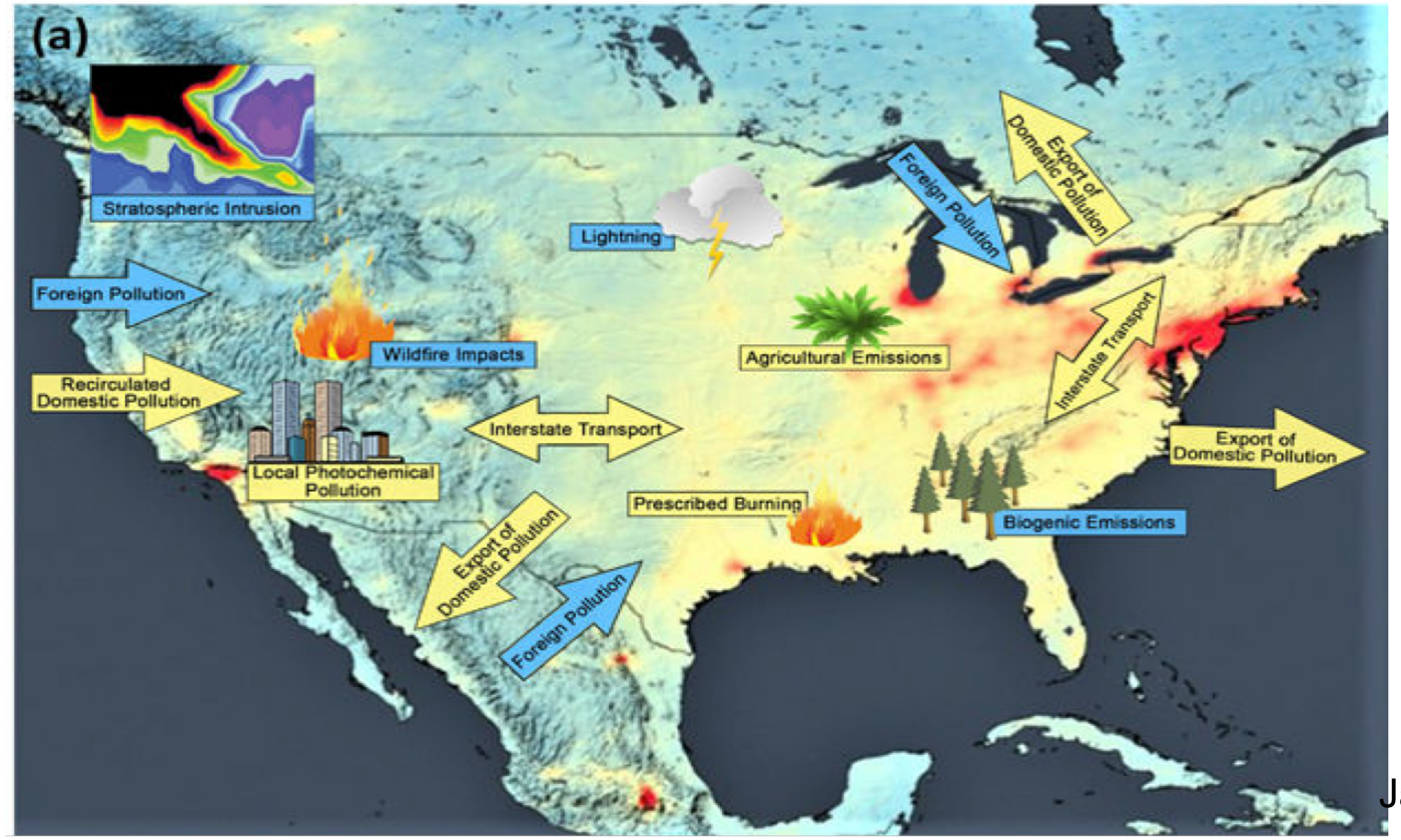
    Data products have been saved in HDF format (same as in NASA EOS L2 products)



HAQAST Tiger Team on background ozone

- Background ozone is the focus of one of four HAQAST Tiger Teams selected for FY19: “Satellite-Evaluated and Satellite-Informed Ozone Distributions for Estimating U.S. Background Ozone”.
- The stakeholder needs addressed by the Background Ozone TT are:
  - Accurate specification of boundary conditions for regulatory air quality and health modeling
  - Reliable estimates of ozone attributable to background sources, including separate quantification of natural ozone and that transported from other nations, particularly during high-ozone episodes

Sources of US Background Ozone



Jaffe et al., 2018

Tiger Team goal and proposed simulations

Goal: improve the quantification of background ozone in SIPs, a critical component of the development of our stakeholders' attainment plans. To do so, we will:

- Provide a coordinated set of boundary conditions for ozone, background ozone (no U.S. anthropogenic emissions), and natural ozone (no global anthropogenic emissions) for 2016 from multiple global models that are evaluated with or informed by satellite data.
- Establish 'best practices' for evaluating models with satellite ozone measurements, and for evaluating satellite-informed simulations with independent datasets such as those from surface stations and ozonesondes.

Deliverable, Milestone	AM3	GEOS-Chem	RAQMs
Boundary Conditions From Satellite-Evaluated Models (Feb 2019)	Fiore	Neu Henze	Pierce
Boundary Conditions from Satellite-Informed Models (Apr 2019)		Neu (OMI NO_2, AIRS/OMI O_3, MLS O_3) Henze (OMI SO_2, NO_2)	Pierce (OMI NO_2, O_3, AIRS CO, MLS O_3, MODIS AOD)
Background and Natural O_3 (U.S. and global Anthropogenic Emissions set to 0) (Apr 2019)	Fiore	Neu (Standard model) Neu (OMI NO_2, MLS O_3) Henze (OMI SO_2, NO_2)	

Summary

- A 13-year tropospheric chemistry reanalysis has been conducted using multi-constituent multi-sensor satellite data assimilation, in order to provide comprehensive information on atmospheric composition variability.
- The reanalysis data, combined with suborbital and ground-based measurements, has been used to improve our understanding of atmospheric composition and their impacts on air quality and climate.
- The observation operators of joint AIRS/OMI data products enable data assimilation, e.g., "CHASER-DA", demonstrating the significant impacts on ozone distributions
- Assimilating datasets from a new constellation of LEO sounders (e.g., IASI, AIRS, CrIS, Sentinel-5p, and Sentinel-5) and GEO satellites (Sentinel-4, GEMS, and TEMPO) will provide more detailed knowledge of ozone and its precursors